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Licensed Application Software

Licensed Application Software: Overview

DRAFT

This article is being reviewed for completeness and technical accuracy.

A few licensed applications from different vendors are installed on NAS HECC systems under the */nasa* directory. They are either purchased by NAS (with justification that many users need it) or by users themselves. If you would like to use a licensed application which is not yet available on NAS HECC systems, you may have to purchase the license yourself.

Tecplot

DRAFT

This article is being reviewed for completeness and technical accuracy.

Tecplot 360 is a CFD and Numerical Simulation Visualization Software used in post-processing simulation results. Common tasks associated with post-processing analysis of flow solver (e.g. Fluent, STAR-CD, OpenFOAM) can include such tasks as:

- Calculating grid quantities (e.g. aspect ratios, skewness, orthogonality and stretch factors)
- Normalizing data; Deriving flow field functions like pressure coefficient or vorticity magnitude
- Verifying solution convergence
- Estimating the order of accuracy of solutions
- Interactively exploring data through cut planes (a slice through a region), iso-surfaces (3-D maps of concentrations), particle paths (dropping an object in the "fluid" and watching where it goes).

As of Dec. 2008, the Tecplot license at NAS no longer has restrictions on the number of copies of Tecplot that can be run concurrently.

Note: If you have set the stacksize with a command like "limit stacksize unlimited", you will have to reduce the stacksize for Tecplot to run. For example,

```
%limit stacksize 2000000
```

For more information, please visit Tecplot's documentation page.

See also:

http://en.wikipedia.org/wiki/Tecplot

IDL

DRAFT

This article is being reviewed for completeness and technical accuracy.

IDL is a software for data analysis, visualization, and cross-platform application development. IDL combines tools for any type of project, from "quick-look," interactive analysis and display to large-scale commercial programming projects.

For more information, please visit the IDL home page.

There are 6 licenses available for 6 users to use IDL at the same time. If you are not able to use idl because the licenses are being used, try using it at a later time, or issue the command 'lmstat -a' to find out how many licenses are in use.

See also:

http://en.wikipedia.org/wiki/IDL_(programming_language)

LS-DYNA

DRAFT

This article is being reviewed for completeness and technical accuracy.

LS-DYNA is a general-purpose transient dynamic finite element program capable of simulating complex real world problems. It is optimized for shared- and distributed-memory Unix, Linux, and Windows based, platforms.

Current license (good until Aug. 31, 2011) allows upto 4 CPUs.

Typical usage:

```
ls971d NCPUS=$OMP_NUM_THREADS I=**.key

mpiexec -np xx mpp971d I=**.key
```

Use the lstc_qrun command to check how many CPUs are using the license. Use the lstc_qkill command to release the license if it is not released automatically after a job is terminated.

For more information, please visit the LS-DYNA web page.

See also:

http://en.wikipedia.org/wiki/LS-DYNA

Matlab

DRAFT

This article is being reviewed for completeness and technical accuracy.

Matlab is a numerical computing environment and programming language. Created by The MathWorks, Matlab allows easy matrix manipulation, plotting of functions and data, implementation of algorithms, creation of user interfaces, and interfacing with programs in other languages. Although it specializes in numerical computing, an optional toolbox interfaces with the Maple symbolic engine, allowing it to be part of a full computer algebra system.

For more information, please visit the Matlab web site at MathWorks.

```
Note: Matlab 2010 does not work on Pleiades or Columbia yet because
of technical issues.
```

See also:

http://en.wikipedia.org/wiki/Matlab

Gaussian

DRAFT

This article is being reviewed for completeness and technical accuracy.

Gaussian 03 is a suite of electronic structure programs. It is used by chemists, chemical engineers, biochemists, physicists and others for research in established and emerging areas of chemical interest.

Starting from the basic laws of quantum mechanics, Gaussian predicts the energies, molecular structures, and vibrational frequencies of molecular systems, along with numerous molecular properties derived from these basic computation types. It can be used to study molecules and reactions under a wide range of conditions, including both stable species and compounds which are difficult or impossible to observe experimentally such as short-lived intermediates and transition structures.

For more information, please see the Gaussian manual or the Gaussian web site.

Two versions (c.02 and e.01) of Gaussian03 have been installed on Columbia systems. To use the older c.02 version, do the following in your PBS script:

```
module load gaussian.03.c02
source $g03root/g03/bsd/g03.login

g03 input output
```

To use the newer e.01 version (built with intel-comp.10.0.023 and intel-mkl.9.1.023), do:

```
module load gaussian.03.e.01
source $g03root/g03/bsd/g03.login

g03 input output
```

If you are a bash user, then do:

```
. /usr/share/modules/init/bash
module load gaussian.03.e.01
. $g03root/g03/bsd/g03.profile

g03 input output
```

See also:

http://en.wikipedia.org/wiki/GAUSSIAN

FieldView

DRAFT

This article is being reviewed for completeness and technical accuracy.

FieldView is Intelligent Light's CFD post-processing software to quickly identify important flow features and characteristics in simulations. It allows interactive exploration for thorough understanding of results. You can use it to examine and compare cases, extract critical values, and make presentations.

Current license allows up to 4 concurrent uses.

For more information, see Intelligent Light's FieldView home page.

Ensight

DRAFT

This article is being reviewed for completeness and technical accuracy.

EnSight is a software package from CEI that is used for analyzing, visualizing and communicating high-end scientific and engineering datasets. It is a post processing environment with an extensive list of features.

Please see the CEI EnSight home page to get more information.

Gridgen

DRAFT

This article is being reviewed for completeness and technical accuracy.

Gridgen is Pointwise's meshing software used by engineers and scientists to generate high quality grids for engineering analysis.

For more information, please visit the Gridgen home page at the Pointwise web site.